The transformation of irreducible tensor operators under spherical functions

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Abstract The irreducible tensor operators and their tensor products employing Racah algebra are studied. Transformation procedure of the coordinate system operators act on are introduced. The rotation matrices and their parametrization by the spherical coordinates of vector in the fixed and rotated coordinate systems are determined. A new way of calculation of the irreducible coupled tensor product matrix elements is suggested. As an example, the proposed technique is applied for the matrix element construction for two electrons in a field of a fixed nucleus.

1 Introduction

The main aim of present work is to parametrize irreducible matrix representation of either $SO(3)$ or $SU(2)$ group by the coordinates of $S^2 \times S^2$, where S^2 denotes the unit 2-dimension sphere. The motivation is grounded on the following occasions: (i) the difficulties in theoretical atomic spectroscopy arising through multiple integrals of N-electron angular parts; (ii) inconvenience of Wigner-Eckart theorem application for irreducible tensor operator matrix elements on the basis of functions, expressed in terms of Wigner D-function.

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In theoretical atomic physics the algorithms of matrix element calculation for atomic quantities on the basis of many-electron wave functions are well known and widely used [1,2]. The construction of matrix element is based on the structure of many-electron function, which is represented by coupled tensor product of one-electron eigenstates. The latter formulation leads to complicated N-electron angular parts and various techniques, in order to simplify the calculation of many-electron matrix element [3,4,5]. According to Racah [6,7], the basis eigenstates ϕ_m^λ behave in the same way as the spherical tensor operators T_m^λ by means of transformations under irreducible matrix representations. The eigenstates ϕ_m^λ of central-field atomic Hamiltonian are usually enunciated by spherical functions on $SO(3)/SO(2)$ quotient group, multiplied by 2×1 spin matrices. However, in [8] it was showed that $\phi\left(\hat{x}_\xi\right) = \phi\left(\theta_\xi, \varphi_\xi\right)$ can be expressed by Wigner $D\left(\bar{\Omega}_\xi\right)$ functions on $SU(2)$, where $\bar{\Omega}_\xi = \left(\Phi_\xi, \Theta_\xi, 0\right) = \left(\varphi_\xi + \pi/2, \theta_\xi, 0\right)$. Furthermore, Bhatia *et al.* in [9] constructed two-electron wave function $\Phi\left(\hat{x}_1, \hat{x}_2\right)$ in terms of the spherical functions $D\left(\Omega\right)$, where Ω, as usually, denotes Euler angles $\left(\Phi, \Theta, \Psi\right)$, i.e., rotation on S^2 from $\hat{x}_1$ to $\hat{x}_2$ and *vice verse*. Unfortunately, it is evident that for this basis the Wigner-Eckart theorem can not be applied directly, what leads to necessity to expand $D\left(\Omega\right)$ over $\hat{x}_1, \hat{x}_2$.

In this work we start from notations in [1], [10]. We express rotation matrix by the spherical coordinates of vector in the fixed and rotated coordinate systems, rather than the rotation angles in an explicit form (Sec. 3 and Sec. 4). Following this route, we demonstrate technique of matrix element construction, when $2N$-integral (over the spherical coordinates θ_ξ, φ_ξ with $\xi = 1, 2, \ldots, N$) is reduced up to a double one (Sec. 6). The technique is based on studied properties of integrity for obtained spherical functions (Sec. 5) and proposed transformation coefficients, called the rotated Clebsch-Gordan coefficients (CGC) or simply RCGC (Sec. 6.1).

2 Preliminaries

The well known transformation formula for k-rank spherical tensor operators T_q^k, $q \in [-k, +k]$, is given by

$$T_q^k\left(K_2\right) = \sum_{q'} D_{qq'}^k\left(\Omega\right) T_{q'}^k\left(K_1\right), \tag{1}$$

where the symbols K_1 and K_2 show that the corresponding tensor operator is defined in the fixed and rotated coordinate system, respectively. The generalized spherical function $D_{qq'}^k$ on $SO(3)$ or $SU(2)$ is of the form [10]

$$D_{qq'}^k\left(\Omega\right) = a\left(k, q, q'\right) e^{i\left(q\Phi + q'\Psi\right)} \left\{\cos\left(\tfrac{1}{2}\Theta\right)\right\}^{2k} \sum_p b_p\left(k, q, q'\right) \left\{\tan\left(\tfrac{1}{2}\Theta\right)\right\}^{2p-q+q'}, \tag{2}$$

$$a\left(k, q, q'\right) = i^{q'-q} \sqrt{(k+q)!\,(k-q)!\,(k+q')!\,(k-q')!}, \tag{3}$$

$$b_p\left(k, q, q'\right) = \frac{(-1)^p}{p!\,(p+q'-q)!\,(k+q-p)!\,(k-q'-p)!}, \tag{4}$$

where $\Phi, \Psi \in [0, 2\pi]$ and $\Theta \in [0, \pi]$. In this work the standard phase system is used in which complex and Hermitian conjugate operators accordingly denote $\overline{D_{qq'}^k} = (-1)^{q-q'} D_{-q-q'}^k$ and $T_q^{k\dagger} = (-1)^{k-q} T_{-q}^k$. It follows from Eq. (1), the rotated coordinate system K_2 depends on the

fixed system K_1 and the rotation angles Ω. Such a dependency can be reformulated in a different way: the rotation angles Ω depend on the coordinates of given (or known) point, located on S^2 in the fixed and rotated coordinate systems. These spherical coordinates will be denoted $\hat{x}_1$ (in K_1) and $\hat{x}_2$ (in K_2). On the other hand, the spherical function D, which depends on Ω, can also be expressed as a function of the variables $\hat{x}_1, \hat{x}_2$. In the next section the latter dependency in an explicit form is presented.

3 The geometry of rotation angles

In order to express the generalized spherical function D by the coordinates $\hat{x}_1$, $\hat{x}_2$ of vector in the fixed and rotated coordinate system, the following geometry is defined. Suppose we have a map $\Omega : S^2 \times S^2 \mapsto SO(3)$. Its representation onto the linear space of vectors $\hat{r}_i = r_i/|r_i| = \left(x_i \ y_i \ z_i \right)^{\mathrm{T}} \in \mathbf{R}^3$ ($|r_i| = \mathrm{const.} \ \forall i \in \mathbb{Z}^+$ - positive integers) is associated in the following way

$$\begin{cases} \hat{r}_2 = R(\Omega)\hat{r}_1, \\ x_i = \sin\theta_i \cos\varphi_i, y_i = \sin\theta_i \sin\varphi_i, z_i = \cos\theta_i, \end{cases} \tag{5}$$

where the coordinate system K_1 is rotated (the ZXZ convention) by the rotation matrix R of $SO(3)$ [10,11]. Then the system of three equations in Eq. (5) is rewritten in the form

$$\begin{cases} x_2 = -x_1' \sin\varphi - u' \cos\varphi, \\ y_2 = x_1' \cos\varphi - u' \sin\varphi, \\ z_2 = y_1' \sin\theta + z_1' \cos\theta, \end{cases} \tag{6}$$

where

$$u' = y_1' \cos\theta - z_1' \sin\theta, \tag{7}$$

$$\begin{cases} x_1' = x_1 \cos\Psi - y_1 \sin\Psi, \\ y_1' = x_1 \sin\Psi + y_1 \cos\Psi, \\ z_1' = z_1. \end{cases} \tag{8}$$

The parameter Ψ is chosen optionally in the range $[0, 2\pi]$. Partial solutions of subsystems (x_2, z_2) and (y_2, z_2) for θ, φ are substituted then in Eq. (2). Optimal values of Ψ are found by solving variational equation, varying obtained spherical function with respect to Ψ (for details see Appendix A). We attain, that solutions in $\mathbb{R}$ satisfy equation

$$\sin\theta_1 \cos(\varphi_1 + \Psi) = 0. \tag{9}$$

The solutions are:

1. $\cos(\varphi_1 + \Psi) = 0 \Rightarrow \Psi = -\varphi_1 + \sigma'\frac{\pi}{2} + \bar{\sigma}\pi + 2\pi n'$, $n' \in \mathbb{Z}^+$, $\sigma' = \pm 1$, $\bar{\sigma} = 0, \pm 1$.
2. $\sin\theta_1 = 0 \quad \forall \Psi \in [0, 2\pi]$.

First of all let us analyze item (1) - the situation when $\sin\theta_1 \neq 0$. Then $y_1' = \sigma' \sin\theta_1$, if $\bar{\sigma} = 0$ and $y_1' = -\sigma' \sin\theta_1$ if $\bar{\sigma} = \pm 1$ (see Eq. (8)). Secondly, when item (2) is valid, we obtain that $\theta_1 = 0$ or $\theta_1 = \pi$. The parameter Ψ then could be of any value in the range $[0, 2\pi]$. It is clear that the solution $\sin\theta_1 = 0$ (item (2)) is a particular case of item (1) if the angle Ψ is chosen to be equal to $\Psi = -\varphi_1 + \sigma'\frac{\pi}{2} + \bar{\sigma}\pi + 2\pi n'$. Since in item (2) the solution

Table 1 The values for the parameters α, β, γ, δ, n

The maps			α	β	γ	δ	n	The maps	α	β	γ	δ	n
$\Omega_1^{\pm}$	Ω_1^+	Ω_{11}^+	+	+	+	−	0	$\Omega_2^{\pm}$					
		Ω_{12}^+	−	+	+	+		Ω_2^+	+	+	−	+	0
	Ω_1^-	Ω_{11}^-	+	−	+	−							
		Ω_{12}^-	−	−	+	+		Ω_2^-	−	−	−	−	1

Ψ can have arbitrary values in the range $[0,2\pi]$, we choose it equal to the solution given by item (1). Consequently, the solutions of the system in Eq. (6) are

$$\Phi = \varphi_2 + \alpha\frac{\pi}{2}, \; \Theta = \beta\left(\theta_1 - \gamma\theta_2\right) + 2\pi n, \; \Psi = -\varphi_1 + \delta\frac{\pi}{2} + 2\pi n', \tag{10}$$

where $n' \in \mathbb{Z}^+$ and the values for α, β, γ, δ, n are presented in Table 1. The function $\Omega(\hat{x}_1, \hat{x}_2)$ may be expanded into several different geometries, representing miscellaneous rotations.

(a) $\theta_1 - \theta_2 \in [0,\pi]$.

$$\varphi_2 \in [0,\pi]: \qquad\qquad\qquad \varphi_2 \in (\pi, 2\pi]:$$

$$\Omega_{11}^+ = \begin{cases} \Phi = \varphi_2 + \frac{\pi}{2}, \\ \Theta = \theta_1 - \theta_2, \\ \Psi = -\varphi_1 - \frac{\pi}{2} \; (2\pi). \end{cases} \qquad \Omega_{12}^+ = \begin{cases} \Phi = \varphi_2 - \frac{\pi}{2}, \\ \Theta = \theta_1 - \theta_2, \\ \Psi = -\varphi_1 + \frac{\pi}{2} \; (2\pi). \end{cases} \tag{11}$$

(b) $\theta_2 - \theta_1 \in [0,\pi]$.

$$\varphi_2 \in [0,\pi]: \qquad\qquad\qquad \varphi_2 \in (\pi, 2\pi]:$$

$$\Omega_{11}^- = \begin{cases} \Phi = \varphi_2 + \frac{\pi}{2}, \\ \Theta = \theta_2 - \theta_1, \\ \Psi = -\varphi_1 - \frac{\pi}{2} \; (2\pi). \end{cases} \qquad \Omega_{12}^- = \begin{cases} \Phi = \varphi_2 - \frac{\pi}{2}, \\ \Theta = \theta_2 - \theta_1, \\ \Psi = -\varphi_1 + \frac{\pi}{2} \; (2\pi). \end{cases} \tag{12}$$

(c) $\theta_1 + \theta_2 \in (0,\pi]$.

$$\Omega_2^+ = \begin{cases} \Phi = \varphi_2 + \frac{\pi}{2}, \\ \Theta = \theta_1 + \theta_2, \\ \Psi = -\varphi_1 + \frac{\pi}{2} \; (2\pi). \end{cases} \tag{13}$$

(d) $\theta_1 + \theta_2 \in [\pi, 2\pi]$.

$$\Omega_2^- = \begin{cases} \Phi = \varphi_2 - \frac{\pi}{2}, \\ \Theta = 2\pi - \theta_1 - \theta_2, \\ \Psi = -\varphi_1 - \frac{\pi}{2} \quad (2\pi). \end{cases} \tag{14}$$

The function $\Omega_1^+ = \left\{\Omega_{11}^+, \Omega_{12}^+\right\}$ is matched for the case when $\theta_1 \geq \theta_2$, while the function $\Omega_1^- = \left\{\Omega_{11}^-, \Omega_{12}^-\right\}$ is matched for the case when $\theta_2 \geq \theta_1$. The functions $\Omega_{11}^{\pm}$ describe rotations for given $\varphi_2 \in [0,\pi]$; according to $\Omega_{12}^{\pm}$, rotations are realized for $\varphi_2 \in (\pi, 2\pi]$. The function $\Omega_2^{\pm} = \left\{\Omega_2^+, \Omega_2^-\right\}$ defines another possible rotation for the given angles $\theta_1 + \theta_2 \in (0,\pi]$ or $\theta_1 + \theta_2 \in [\pi, 2\pi]$. Note, if $\varphi_2 \in \left[\frac{3\pi}{2}, 2\pi\right]$, then for the rotation Ω_2^+, the angle $\Phi > 2\pi$. On the other hand, rotation over the angle 2π geometrically is equivalent to initial state. Thus, one can choose whether $\Phi > 2\pi$ or $0 < \Phi - 2\pi < 2\pi$. The same idea is valid and for the rotation Ω_2^-. Finally, when $\theta_1 = \theta_2 = 0$, the angle $\Theta = 0$ and the angles Φ, Ψ acquire

any values in $[0, 2\pi]$. Then the rotation matrix $R(\Omega) = R_z(\Phi + \Psi)$. Hence, in this case the full rotation is made by the angle $\Phi + \Psi$ around the z-axis. In other words, if $\theta_1 = \theta_2 = 0$, rotation by the Euler angles Ω is not singularly defined. Further it will be assumed that θ_1 and θ_2 are not equal to zero at the same time (that is why the range of $\theta_1 + \theta_2$ for Ω_2^+ is open from the left).

4 Spherical functions

In the previous section the mapping from $S^2 \times S^2$ to $SO(3)$ has been defined. It was demonstrated that possible rotations in $\mathbf{R}^3$ from K_1 to K_2 could be realized by the rotation angles $\Omega_1^{\pm} = \{\Omega_1^+, \Omega_1^-\} = \{\Omega_{11}^+, \Omega_{12}^+, \Omega_{11}^-, \Omega_{12}^-\}$ and $\Omega_2^{\pm} = \{\Omega_2^+, \Omega_2^-\}$. If substituting these functions in Eq. (2), we would obtain the following spherical function (for alternative expressions, see Appendix B)

$$\left(n, n'; \alpha, \beta, \gamma, \delta | \hat{x}_1, \hat{x}_2\right)_{qq'}^k = i^{\alpha q + \delta q'} (-1)^{2\left(nk + n'q'\right)} \beta^{q'-q} a\left(k, q, q'\right) e^{i\left(q\varphi_2 - q'\varphi_1\right)}$$

$$\times \left\{\cos\left[\tfrac{1}{2}\left(\theta_1 - \gamma\theta_2\right)\right]\right\}^{2k} \sum_p b_p\left(k, q, q'\right) \left\{\tan\left[\tfrac{1}{2}\left(\theta_1 - \gamma\theta_2\right)\right]\right\}^{2p+q'-q}, \tag{15}$$

where $k \in \mathbb{Z}^+, \mathbb{Q}^+$ and $\mathbb{Q}^+ = \{m + 1/2; m \in \mathbb{Z}^+\}$; the indices $q, q' \in [-k, +k]$. Let us define particular cases of Eq. (15) in the following way

$$\left(0, n'; +, \pm, +, - | \hat{x}_1, \hat{x}_2\right)_{qq'}^k = {}^{\pm}\xi_{qq'}^k\left(\hat{x}_1, \hat{x}_2\right), \tag{16}$$

$$\left(0, n'; -, \pm, +, + | \hat{x}_1, \hat{x}_2\right)_{qq'}^k = {}^{\pm}\vartheta_{qq'}^k\left(\hat{x}_1, \hat{x}_2\right) = (-1)^{q'-q} {}^{\pm}\xi_{qq'}^k\left(\hat{x}_1, \hat{x}_2\right), \tag{17}$$

$$\left(0, n'; +, +, -, + | \hat{x}_1, \hat{x}_2\right)_{qq'}^k = {}^{+}\zeta_{qq'}^k\left(\hat{x}_1, \hat{x}_2\right), \tag{18}$$

$$\left(1, n'; -, -, -, - | \hat{x}_1, \hat{x}_2\right)_{qq'}^k = {}^{-}\zeta_{qq'}^k\left(\hat{x}_1, \hat{x}_2\right) = (-1)^{2q'} {}^{+}\zeta_{qq'}^k\left(\hat{x}_1, \hat{x}_2\right), \tag{19}$$

and the matrices

$$\Omega_1^{\pm}: {}^{\pm}\eta^k\left(\hat{x}_1, \hat{x}_2\right) \in \left\{{}^{\pm}\xi^k\left(\hat{x}_1, \hat{x}_2\right), {}^{\pm}\vartheta^k\left(\hat{x}_1, \hat{x}_2\right)\right\}. \tag{20}$$

It is seen, the spherical functions ${}^{\pm}\eta_{qq'}^k\left(\hat{x}_1, \hat{x}_2\right)$ and ${}^{\pm}\zeta_{qq'}^k\left(\hat{x}_1, \hat{x}_2\right)$ are the generalized spherical functions $D_{qq'}^k\left(\Omega_1^{\pm}\right)$ and $D_{qq'}^k\left(\Omega_2^{\pm}\right)$ parametrized by the coordinates of $S^2 \times S^2$, respectively. Particularly, the matrix ${}^{+}\eta^k\left(\hat{x}_1, \hat{x}_2\right)$ represents rotation in $\mathbf{R}^3$ from K_1 to K_2, when $\theta_1 \geq \theta_2$ and it is associated to the map Ω_1^+, while the matrix ${}^{-}\eta^k\left(\hat{x}_1, \hat{x}_2\right)$ describes rotation from K_1 to K_2 when $\theta_2 \geq \theta_1$ and it is associated to the map Ω_1^-. The matrices ${}^{+}\zeta^k\left(\hat{x}_1, \hat{x}_2\right)$ and ${}^{-}\zeta^k\left(\hat{x}_1, \hat{x}_2\right)$ are related to the maps Ω_2^+ and Ω_2^-.

In accordance with Eqs. (16)-(19), the spherical functions ${}^{\pm}\xi, {}^{\pm}\vartheta$ and ${}^{\pm}\zeta$ are connected to each other as follows

$$\begin{aligned} {}^{-}\xi_{qq'}^k &= (-1)^{q'-q} {}^{+}\xi_{qq'}^k, & {}^{-}\vartheta_{qq'}^k &= (-1)^{q'-q} {}^{+}\vartheta_{qq'}^k, \\ {}^{+}\vartheta_{qq'}^k &= {}^{-}\xi_{qq'}^k, & {}^{-}\zeta_{qq'}^k &= (-1)^{2q'} {}^{+}\zeta_{qq'}^k. \end{aligned} \tag{21}$$

It directly follows from Eq. (21), that

$$^{+}\eta_{qq'}^{k} = {}^{-}\eta_{qq'}^{k} = \eta_{qq'}^{k} \in \left\{ {}^{+}\xi_{qq'}^{k}, {}^{-}\xi_{qq'}^{k} \right\}, \qquad {}^{-}\xi_{qq'}^{k} = \overline{{}^{+}\xi_{-q-q'}^{k}}, \tag{22}$$

where the column vectors of $^{\pm}\xi^{k}$ are orthonormal, i.e.,

$$\sum_{q} {}^{+}\xi_{qq'}^{k} {}^{-}\xi_{-q-q''}^{k} = \delta_{q'q''}. \tag{23}$$

The latter condition is, of course, valid and for the rest of spherical functions.

It is noticeable, the matrices η^{k} and $^{\pm}\zeta^{k}$ are the unitary irreducible matrix representations of $SO(3)$ (for $k \in \mathbb{Z}^{+}$) or of $SU(2)$ (for $k \in \mathbb{Q}^{+}$), parametrized by the coordinates of $S^{2} \times S^{2}$. Hence, the irreducible tensor operators T_{q}^{k} transform among themselves as follows (to compare, see Eq. (1))

$$\begin{aligned} \Omega_{1}^{\pm} &: T_{q}^{k}(K_{2}) = \sum_{q'} \eta_{qq'}^{k}(\hat{x}_{1}, \hat{x}_{2}) T_{q'}^{k}(K_{1}), \\ \Omega_{2}^{\pm} &: T_{q}^{k}(K_{2}) = \sum_{q'} {}^{\pm}\zeta_{qq'}^{k}(\hat{x}_{1}, \hat{x}_{2}) T_{q'}^{k}(K_{1}). \end{aligned} \tag{24}$$

The transformation formula for the maps $\Omega_{1}^{\pm}$ is restricted by the condition $\theta_{1} \neq \theta_{2}$. In a contrary case, only the maps $\Omega_{2}^{\pm}$ are valid. Consequently, the reduction formulas for the spherical functions

$$^{\pm}\tau_{qq'}^{k}(.,.) \in \left\{ \eta_{qq'}^{k}(.,.), {}^{\pm}\zeta_{qq'}^{k}(.,.) \right\} \tag{25}$$

are these

$$^{\pm}\tau_{q_{1}q_{1}'}^{k_{1}}(.,.) \, {}^{\pm}\tau_{q_{2}q_{2}'}^{k_{2}}(.,.) = \sum_{k} {}^{\pm}\tau_{qq'}^{k}(.,.) \begin{bmatrix} k_{1} & k_{2} & k \\ q_{1} & q_{2} & q \end{bmatrix} \begin{bmatrix} k_{1} & k_{2} & k \\ q_{1}' & q_{2}' & q' \end{bmatrix}, \tag{26}$$

where in the brackets $(.,.)$ the spherical coordinates of $S^{2} \times S^{2}$ are given. The Clebsch-Gordan coefficients of $SU(2)$ are none zero only when $q = q_{1} + q_{2}$ and $q' = q_{1}' + q_{2}'$. The summation is performed over $k = |k_{1} - k_{2}|, |k_{1} - k_{2}| + 1, \ldots, k_{1} + k_{2}$.

Example. Suppose, $\hat{x}_{1} = \left(\frac{\pi}{6}, \frac{\pi}{4} \right)$ and $\hat{x}_{2} = \left(\frac{\pi}{3}, \pi \right)$. Possible rotations are realized then in accordance with $\Omega_{11}^{-} = \left(\frac{3\pi}{2}, \frac{\pi}{6}, \frac{5\pi}{4} \right)$, $\Omega_{2}^{+} = \left(\frac{3\pi}{2}, \frac{\pi}{2}, \frac{\pi}{4} \right)$. Transformation formulas in Eq. (24) are valid for the spherical functions $^{-}\xi_{qq'}^{k} \left(\frac{\pi}{6}, \frac{\pi}{4}, \frac{\pi}{3}, \pi \right)$ and $^{+}\zeta_{qq'}^{k} \left(\frac{\pi}{6}, \frac{\pi}{4}, \frac{\pi}{3}, \pi \right)$ which coequal to $D_{qq'}^{k} \left(\frac{3\pi}{2}, \frac{\pi}{6}, \frac{5\pi}{4} \right)$ and $D_{qq'}^{k} \left(\frac{3\pi}{2}, \frac{\pi}{2}, \frac{\pi}{4} \right)$. Suppose $k = \frac{5}{2}$ and $q = -\frac{1}{2}, q' = \frac{3}{2}$. Then

$$^{-}\xi_{-\frac{1}{2}\frac{3}{2}}^{\frac{5}{2}} \left(\frac{\pi}{6}, \frac{\pi}{4}, \frac{\pi}{3}, \pi \right) = D_{-\frac{1}{2}\frac{3}{2}}^{\frac{5}{2}} \left(\frac{3\pi}{2}, \frac{\pi}{6}, \frac{5\pi}{4} \right) = \frac{(-1)^{\frac{1}{8}}}{32} \left(13 - 3\sqrt{3} \right),$$

$$^{+}\zeta_{-\frac{1}{2}\frac{3}{2}}^{\frac{5}{2}} \left(\frac{\pi}{6}, \frac{\pi}{4}, \frac{\pi}{3}, \pi \right) = D_{-\frac{1}{2}\frac{3}{2}}^{\frac{5}{2}} \left(\frac{3\pi}{2}, \frac{\pi}{2}, \frac{\pi}{4} \right) = \frac{(-1)^{\frac{5}{8}}}{4}.$$

One may notice, according to expressions in Eq. (21), it is possible to find out how all other spherical functions are related to the calculated functions above.

5 The integral of spherical functions

The choice of geometries $\Omega_1^\pm$, $\Omega_2^\pm$ is convenient for other applications of obtained spherical functions $\pm\tau_{qq'}^k$. This is because the parameters θ_1, θ_2 and φ_1, φ_2 are separated. Consequently, the functions which depend on these parameters can be integrated separately, i.e., the integral on S^2 is naturally separated into the integrals over φ_i and over θ_i. By definition, the functions $\pm\tau_{qq'}^k(\hat{x}_1, \hat{x}_2)$ are determined in different areas $L^2(\Omega) \subset S^2$, which restrict the existence of integrity. Therefore, we construct the integral

$$\mathscr{S}_{qq'}^k(\hat{x}_1; \gamma) = \int_{S^2} \mathrm{d}\hat{x}_2 \left(n, n'; \alpha, \beta, \gamma, \delta | \hat{x}_1, \hat{x}_2\right)_{qq'}^k. \tag{27}$$

Suppose, $\gamma = +1$, i.e., the map $\Omega_1^\pm$ is realized. Let the areas (or paths of integration) on S^2 to be

$$L^2\left(\Omega_{11}^+\right) = \{\varphi_2 \in [0, \pi]; \theta_2 \in [0, \theta_1]\}, \ L^2\left(\Omega_{12}^+\right) = \{\varphi_2 \in [\pi, 2\pi]; \theta_2 \in [0, \theta_1]\},$$
$$L^2\left(\Omega_{11}^-\right) = \{\varphi_2 \in [0, \pi]; \theta_2 \in [\theta_1, \pi]\}, \ L^2\left(\Omega_{12}^-\right) = \{\varphi_2 \in [\pi, 2\pi]; \theta_2 \in [\theta_1, \pi]\}. \tag{28}$$

Here $\Omega_{11}^\pm$ and $\Omega_{12}^\pm$ mark the existence of integrable spherical functions $\pm\xi_{qq'}^k(\hat{x}_1, \hat{x}_2)$ in the corresponding areas $L^2\left(\Omega_{11}^\pm\right)$ and $L^2\left(\Omega_{12}^\pm\right)$. The parameters α, β, γ, δ, n are determined then according to the values presented in Table 1 and the equations in Eq. (10). It is clear, the spherical function $+\xi$ is integrable in $L^2\left(\Omega_{11}^+\right)$ with $n' \in \{1, 2\}$ and in $L^2\left(\Omega_{12}^-\right)$ with $n' \in \{0, 1\}$; the function $-\xi$ is integrable in $L^2\left(\Omega_{11}^-\right)$ with $n' \in \{1, 2\}$ and in $L^2\left(\Omega_{12}^+\right)$ with $n' \in \{0, 1\}$. But $-\xi_{qq'}^k = (-1)^{q'-q} \, {}^+\xi_{qq'}^k$ (see Eq. (21)). This implies

$$\begin{aligned}
\mathscr{S}_{qq'}^k(\hat{x}_1; +) &= \int_{L^2\left(\Omega_{11}^+\right)} \mathrm{d}\hat{x}_2 \, {}^+\xi_{qq'}^k(\hat{x}_1, \hat{x}_2) + \int_{L^2\left(\Omega_{11}^-\right)} \mathrm{d}\hat{x}_2 \, {}^-\xi_{qq'}^k(\hat{x}_1, \hat{x}_2) \\
&+ \int_{L^2\left(\Omega_{12}^+\right)} \mathrm{d}\hat{x}_2 \, {}^-\xi_{qq'}^k(\hat{x}_1, \hat{x}_2) + \int_{L^2\left(\Omega_{12}^-\right)} \mathrm{d}\hat{x}_2 \, {}^+\xi_{qq'}^k(\hat{x}_1, \hat{x}_2) \\
&= \lambda_{q'}(\varphi_1) \, \mathrm{i}^{q-q'-1} \frac{(-1)^q - 1}{q} \left((-1)^{q'} + 1\right) a(k, q, q') \, \mathrm{e}^{-\mathrm{i}q'\varphi_1} \\
&\times \sum_p b_p(k, q, q') \left({}_p I_{qq'}^k(\theta_1; +; 0, \theta_1) + (-1)^{q-q'} {}_p I_{qq'}^k(\theta_1; +; \theta_1, \pi)\right),
\end{aligned} \tag{29}$$

$$\lambda_{q'}(\varphi_1) = \begin{cases} (-1)^{q'}, & \varphi_1 \in \left[0, \frac{\pi}{2}\right], \\ (-1)^{2q'}, & \varphi_1 \in \left(\frac{\pi}{2}, \frac{3\pi}{2}\right], \\ (-1)^{3q'}, & \varphi_1 \in \left(\frac{3\pi}{2}, 2\pi\right]. \end{cases} \tag{30}$$

The definition of ${}_p I_{qq'}^k$ is given by the formula

$$_p I_{qq'}^k(\theta_1; \gamma; a, b) = \int_a^b \mathrm{d}\theta_2 \, \sin\theta_2 \left\{\cos\left[\tfrac{1}{2}(\theta_1 - \gamma\theta_2)\right]\right\}^{2k} \left\{\tan\left[\tfrac{1}{2}(\theta_1 - \gamma\theta_2)\right]\right\}^{2p+q'-q}. \tag{31}$$

For $\gamma = +1$ the integration is performed making the change of integrand $z = \tan[(\theta_1 - \theta_2)/2]$. After some ordinary trigonometric manipulations it acquires the form

$$_p I_{qq'}^k(\theta_1; +; a, b) = 2\left\{2I_1^{p+}(a, b)\cos\theta_1 + \left(I_2^{p+}(a, b) - I_0^{p+}(a, b)\right)\sin\theta_1\right\}, \tag{32}$$

$$I_s^{p+}(a, b) = I_s^{p+}\left(\tan\frac{\theta_1 - b}{2}\right) - I_s^{p+}\left(\tan\frac{\theta_1 - a}{2}\right) \tag{33}$$

with $s = 0, 1, 2$ and $I_s^{p+}(z)$ defined by

$$I_s^{p+}(z) = \int_{\mathbb{R}} dz \, \frac{z^{2p+q'-q+s}}{(1+z^2)^{k+2}} = \frac{z^{2p+q'-q+s+1}}{2p+q'-q+s+1}$$

$$\times \; {}_2F_1 \left(\frac{2p+q'-q+s+1}{2}, k+2; \frac{2p+q'-q+s+3}{2}; -z^2 \right) + \text{const.}, \qquad (34)$$

where ${}_2F_1$ denotes Gauss hypergeometric function.

When $\theta_1 = 0$ or $\theta_1 = \pi$, the function $I_s^{p+}(0, \pi)$ depends on infinite variables ($z = \pm\infty$). For this reason bellow the boundary values of ${}_pI_{qq'}^k(\theta; +; 0, \pi)$ are presented.

1. $\theta = 0$. Then ${}_pI_{qq'}^k(0; +; 0, \pi) = 4I_1^{p+}(-\infty)$ (since $I_1^{p+}(0) = 0$), where

$$I_1^{p+}(-\infty) = \frac{(-1)^{q'-q}}{2} B \left(k+1-p+\frac{q-q'}{2}, 1+p+\frac{q'-q}{2} \right) \qquad (35)$$

   with B being Beta function.
2. $\theta = \pi$. Then

$$_pI_{qq'}^k(\pi; +; 0, \pi) = (-1)^{q-q'} \, _pI_{qq'}^k(0; +; 0, \pi). \qquad (36)$$

For example, it directly follows from Eqs. (31), (36), that

$$I_2 = \int_0^\pi d\theta \, \sin^{2k+1}\theta \, \cos^\gamma \theta = \left[1 + (-1)^\gamma \right] I_1^p(\infty), \qquad (37)$$

$$I_1^p(\infty) = \frac{1}{2} B \left(k+1, \frac{\gamma+1}{2} \right), \qquad (38)$$

where the left hand side of I_2 is the same integral discussed by Pinchon $et\ al.$ [12] (Eqs. (19)-(20)), when developing rotation matrices for real spherical harmonics.

When $k \in \mathbb{Z}^+$, the integral of the spherical function η acquires the form

$$\mathscr{S}_{qq'}^k(\hat{x}_1; +) = \delta_{q0} \pi i^{-q'} \left((-1)^{q'} + 1 \right) a(k, 0, q') e^{-iq'\varphi_1}$$

$$\times \sum_p b_p(k, 0, q') \, _pI_{0q'}^k(\theta_1; +; 0, \pi). \qquad (39)$$

Hence, for integer k, the integral of $(0, n'; \alpha, \beta, +, \delta | \hat{x}_1, \hat{x}_2)_{qq'}^k$ is none zero only if $q = 0$ and q' is even. Particularly, $\mathscr{S}_{00}^0(\hat{x}_1; +) = 4\pi$.

Finally, the integration of $(n, n'; \alpha, \beta, -, \delta | \hat{x}_1, \hat{x}_2)_{qq'}^k$ must be proceeded. For the maps $\Omega_2^\pm$ there is no difference which value of θ_1 and θ_2 is greater or less (or equal). It has been demonstrated earlier, that for Ω_2^+ the condition $0 \leq \theta_1 + \theta_2 \leq \pi$ ($\alpha = \beta = \delta = +$, $n = 0$) must be satisfied, while for Ω_2^- the restriction is: $\pi \leq \theta_1 + \theta_2 \leq 2\pi$ ($\alpha = \beta = \delta = -$, $n = 1$). But when integrating $^\pm\zeta_{qq'}^k(\hat{x}_1, \hat{x}_2)$ over θ_2, the angle θ_2 acquires all values in $[0, \pi]$. This means the map Ω_2^+ is valid only if $\theta_1 = 0$ and the map Ω_2^- is realized only for $\theta_1 = \pi$. Hence, the integration of $^\pm\zeta_{qq'}^k(\hat{x}_1, \hat{x}_2)$ can not be correctly performed for any values of θ_1, except for $\theta_1 = 0$ or $\theta_1 = \pi$. In other words, the spherical functions $^\pm\zeta_{qq'}^k(\hat{x}_1, \hat{x}_2)$, which represent rotations $\Omega_2^\pm$, are not integrable on S^2, in general. For this reason we conclude, that the most preferable spherical functions (at least for integration) are $\eta_{qq'}^k(\hat{x}_1, \hat{x}_2)$, i.e., those

which represent geometries $\Omega_1^{\pm}$. Note, the angles (θ_1, φ_1) and (θ_2, φ_2) are fully determined on S^2 for the maps $\Omega_1^{\pm}$. This implies that for any values of θ_1, φ_1, θ_2, φ_2 there will always exist at least one rotation from the set $\Omega_1^{\pm} = \{\Omega_{11}^{\pm}, \Omega_{12}^{\pm}\}$. Consequently, the loss of geometry $\Omega_2^{\pm}$ does not imply the loss of generality by means of the existence of at least one spherical function from the set $\{^+\xi, {}^-\xi\}$.

6 RCGC technique

Since the irreducible matrix representations $\eta^{\lambda}(\hat{x}_1, \hat{x}_2)$ depend on known coordinates $\hat{x}_1$ and $\hat{x}_2$, it is worth to exploit them in the study of tensor products of irreducible tensor operators T (or basis functions ϕ) directly, but not formally, as in most cases, when tensor operators are transformed under representations $D^{\lambda}(\Omega)$. Moreover, most of the physical operators T_q^k, basically studied in atomic spectroscopy, are expressed in terms of D and their various combinations. These are, for example, the spherical operators $C_q^k(\hat{x}) = i^k D_{q0}^k(\bar{\Omega})$, the spherical harmonics $Y_q^k(\hat{x}) = \sqrt{(2k+1)/4\pi} C_q^k(\hat{x})$. Expressions over D of other operators, such as spin operator S^1, angular momentum operator L^1, can be found, for instance, in [8]. All these mentioned operators also transform among themselves according to Eq. (24). Hence, it is natural for such operators to write $T(\hat{x})$ instead of $T(K)$, which is a general case. We say the operator $T(\hat{x})$ acts on $\hat{x}$ coordinate. Below the latter notation will be used.

6.1 Transformation coefficients

Reduction formula for tensor product reads (see Eq. (24))

$$T_{m_1}^{\lambda_1}(\hat{x}_1) T_{m_2}^{\lambda_2}(\hat{x}_2) = \sum_{\lambda} \bar{T}_m^{\lambda}(\hat{x}_1) c_{m_1 m_2 m}^{\lambda_1 \lambda_2 \lambda}(\hat{x}_1, \hat{x}_2), \tag{40}$$

In this paper the so-called for simplicity rotated Clebsch-Gordan coefficient of the first type or simply RCGC I is defined by

$$c_{m_1 m_2 m}^{\lambda_1 \lambda_2 \lambda}(\hat{x}_1, \hat{x}_2) = \sum_{m_2'} \eta_{m_2 m_2'}^{\lambda_2}(\hat{x}_1, \hat{x}_2) \begin{bmatrix} \lambda_1 & \lambda_2 & \lambda \\ m_1 & m_2' & m \end{bmatrix}, \tag{41}$$

From Eq. (40) we obtain the next expression

$$\bar{\bar{T}}_m^{\lambda}(\hat{x}_1, \hat{x}_2) = \sum_{\lambda' m'} C_{m' m}^{\lambda_1 \lambda_2 \lambda' \lambda}(\hat{x}_1, \hat{x}_2) \bar{T}_{m'}^{\lambda'}(\hat{x}_1), \tag{42}$$

where rotated Clebsch-Gordan coefficient of the second type or simply RCGC II is

$$C_{m' m}^{\lambda_1 \lambda_2 \lambda' \lambda}(\hat{x}_1, \hat{x}_2) = \sum_{m_1 m_2} c_{m_1 m_2 m'}^{\lambda_1 \lambda_2 \lambda'}(\hat{x}_1, \hat{x}_2) \begin{bmatrix} \lambda_1 & \lambda_2 & \lambda \\ m_1 & m_2 & m \end{bmatrix}. \tag{43}$$

Irreducible tensor operators $\bar{T}_m^{\lambda}(\hat{x}_1)$ and $\bar{\bar{T}}_m^{\lambda}(\hat{x}_1, \hat{x}_2)$ are delivered by applying reduction rules for the Kronecker product $\lambda_1 \times \lambda_2 \to \lambda$. However, $\bar{T}_m^{\lambda}$ acts on $\hat{x}_1$, while $\bar{\bar{T}}_m^{\lambda}$ acts on $\hat{x}_1, \hat{x}_2$. For example, if T represents normalized spherical harmonic C, then coupled tensor product $\bar{T}_m^{\lambda}(\hat{x}_1) = i^{\lambda_1 + \lambda_2 - \lambda} C_m^{\lambda}(\hat{x}_1) \begin{bmatrix} \lambda_1 & \lambda_2 & \lambda \\ 0 & 0 & 0 \end{bmatrix}$. Contrarily, tensor operator $\bar{\bar{T}}_m^{\lambda}(\hat{x}_1, \hat{x}_2)$ can not be reduced into one C_m^{λ} due to different spaces, in which $T_{m_i}^{\lambda_i}(\hat{x}_i)$ $(i = 1, 2)$ act on.

Another useful circumstance for RCGC application is based on a possibility to reduce these coefficients. In accordance with Eq. (26), we directly attain

$$c^{\lambda_1\lambda_2\lambda}_{m_1\bar{m}_2 m}(.,.)c^{\bar{\lambda}_1\bar{\lambda}_2\bar{\lambda}}_{\bar{m}_1\bar{m}_2\bar{m}}(.,.) = \sum_{\Lambda_2}\eta^{\Lambda_2}_{M_2 M_2'}(.,.)\sum_{m_2'\bar{m}_2'}\begin{bmatrix}\lambda_1 & \lambda_2 & \lambda \\ m_1 & m_2' & m\end{bmatrix}\begin{bmatrix}\bar{\lambda}_1 & \bar{\lambda}_2 & \bar{\lambda} \\ \bar{m}_1 & \bar{m}_2' & \bar{m}\end{bmatrix}$$

$$\times\begin{bmatrix}\lambda_2 & \bar{\lambda}_2 & \Lambda_2 \\ m_2 & \bar{m}_2 & M_2\end{bmatrix}\begin{bmatrix}\lambda_2 & \bar{\lambda}_2 & \Lambda_2 \\ m_2' & \bar{m}_2' & M_2'\end{bmatrix}. \tag{44}$$

Combining Eqs. (43)-(44), we may also derive reduction formula for RCGC II. It is obvious, demonstrated reduction procedure (see Eq. (42)) can be extended and for many-electron wave functions.

Suppose, for instance, one needs to calculate matrix element of $T_q^k(\hat{x})$ on the basis of eigenfunctions $Y_m^l(\hat{x})$, described on $SO(3)/SO(2)$. The application of RCGC technique directly indicates, that in present case

$$[l\|T^k\|\bar{l}] = i^{\bar{l}-l}[(2\bar{l}+1)/(2l+1)]^{1/2}T_0^k(\hat{0})\begin{bmatrix}\bar{l} & k & l \\ 0 & 0 & 0\end{bmatrix}. \tag{45}$$

The proof is produced in Appendix C. Here it is assumed $\hat{0}\equiv(0,0)$. Reduced matrix element $[l\|T^k\|\bar{l}]$ is obtained from Wigner-Eckart theorem $\langle lm|T_q^k|\bar{l}\bar{m}\rangle = (-1)^{2k}[l\|T^k\|\bar{l}]\begin{bmatrix}\bar{l} & k & l \\ \bar{m} & q & m\end{bmatrix}$. Particularly, if $T^k = C^k$, then operator $T_0^k(\hat{0}) = i^k$, and obtained formula is in fully consistence with Eq. (2.52) in [2]. Thus, Eq. (45) is a generalization of this special case. Going on this route, one can derive matrix element expressions on the basis of more complex eigenfunctions.

One can see from Eq. (42), the specific feature of technique, based on coordinate transformations (or simply RCGC technique), is that tensor structure of operator and wave functions is preserved, and the resultant matrix element is calculated on the basis of transformed operators $\bar{T}(\hat{x})$, i.e., the calculation of multiple integrals transforms to the calculation of a single integral (over $\hat{x}$). This is because each N-electron matrix element

$$\int_{S2}d\hat{x}_1\int_{S2}d\hat{x}_2\ldots\int_{S2}d\hat{x}_N\,\Phi_M^{\Lambda^{bra}\dagger}(\hat{x}_1,\hat{x}_2,\ldots,\hat{x}_N)$$
$$\times T_Q^K(\hat{x}_1,\hat{x}_2,\ldots,\hat{x}_N)\Phi_{M'}^{\Lambda^{ket}}(\hat{x}_1,\hat{x}_2,\ldots,\hat{x}_N)$$

is transformed to

$$\int_{S2}d\hat{x}_1\,\bar{\Phi}_m^{\lambda^{bra}\dagger}(\hat{x}_1)\bar{T}_q^k(\hat{x}_1)\bar{\Phi}_{m'}^{\lambda^{ket}}(\hat{x}_1)$$
$$\times\int_{S2}d\hat{x}_2\int_{S2}d\hat{x}_3\ldots\int_{S2}d\hat{x}_N\,\overline{\eta^{\lambda_2^{bra}}_{m_2\mu_2}(\hat{x}_1,\hat{x}_2)}\,\overline{\eta^{\lambda_3^{bra}}_{m_3\mu_3}(\hat{x}_1,\hat{x}_3)}\ldots\overline{\eta^{\lambda_N^{bra}}_{m_N\mu_N}(\hat{x}_1,\hat{x}_N)}$$
$$\times\eta^{k_2}_{q_2\pi_2}(\hat{x}_1,\hat{x}_2)\eta^{k_3}_{q_3\pi_3}(\hat{x}_1,\hat{x}_3)\ldots\eta^{k_N}_{q_N\pi_N}(\hat{x}_1,\hat{x}_N)$$
$$\times\eta^{\lambda_2^{ket}}_{m_2'\mu_2}(\hat{x}_1,\hat{x}_2)\eta^{\lambda_3^{ket}}_{m_3'\mu_3}(\hat{x}_1,\hat{x}_3)\ldots\eta^{\lambda_N^{ket}}_{m_N'\mu_N}(\hat{x}_1,\hat{x}_N),$$

where $\bar{\Phi}$ and $\bar{T}$ indicate coupled tensor products of $\phi^{\lambda_i}(\hat{x}_1)$ and $T^{k_i}(\hat{x}_1)$, respectively. The application of Eq. (26) for all $\overline{\eta^{\lambda_\xi^{bra}}_{m_\xi\mu_\xi}(\hat{x}_1,\hat{x}_\xi)}$, $\eta^{k_\xi}_{q_\xi\pi_\xi}(\hat{x}_1,\hat{x}_\xi)$, $\eta^{\lambda_\xi^{ket}}_{m_\xi'\mu_\xi'}(\hat{x}_1,\hat{x}_\xi)$, $\xi=2,3,\ldots,N$ implies, that initially determined $2N$-integral reduces to a double one

$$\int_{S2}d\hat{x}_1\,\bar{\Phi}_m^{\lambda^{bra}\dagger}(\hat{x}_1)\bar{T}_q^k(\hat{x}_1)\mathscr{S}^{\Lambda_2}_{M_2 M_2'}(\hat{x}_1;+)\mathscr{S}^{\Lambda_3}_{M_3 M_3'}(\hat{x}_1;+)\ldots\mathscr{S}^{\Lambda_N}_{M_N M_N'}(\hat{x}_1;+)\bar{\Phi}_{m'}^{\lambda^{ket}}(\hat{x}_1).$$

Instead of that, for given N-electron wave functions we produce $N-1$ functions $\mathscr{S}$ (see Eq. (29)) and a product of momenta coupling coefficients (CGC), which can be decomposed into $3nj$-coefficients, if summing over projections.

6.2 Example

A simple application of RCGC technique can be demonstrated, for example, in a study of two electrons, located in some external field (of fixed nucleus, for instance). We refer to [9], where a two-electron wave function is presented by

$$\Psi_m^l(\boldsymbol{r}_1,\boldsymbol{r}_2)=\sum_\mu g_\mu^l(r_1,r_2,\theta_{12})D_{m\mu}^l(\boldsymbol{\Omega}),\qquad(46)$$

with $r_i=|\boldsymbol{r}_i|$; $l\in\mathbb{Z}^+$. In the same paper (Bhatia *et al.* [9]) it was determined, that Laplacian, involving θ_{12} (the angle between vectors $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$), does not affect the orbital angular momentum $l>0$. Thus we may assume, that g is a radial function not going into a deeper analysis, since our aim is the angular part. Then Ψ_m^l may be rewritten as follows

$$\Psi_m^l(\boldsymbol{r}_1,\boldsymbol{r}_2)=\sum_\mu g_\mu^l(r_1,r_2,\theta_{12})\,\eta_{m\mu}^l(\hat{x}_1,\hat{x}_2).\qquad(47)$$

Suppose we want to calculate the Coulomb $1/r_{12}$ matrix element. In this case the interaction in a tensor form reads $T_0^0(\boldsymbol{r}_1,\boldsymbol{r}_2)=\sum_k(r_<^k/r_>^{k+1})\left(C^k(\hat{x}_1)\cdot C^k(\hat{x}_2)\right)$, where $r_<=\min(r_1,r_2)$ and $r_>=\max(r_1,r_2)$. The scalar product $\left(C^k(\hat{x}_1)\cdot C^k(\hat{x}_2)\right)$ is reduced in agreement with Eq. (42), what leads to the following construction of $\langle\Psi_m^l|r_{12}^{-1}|\Psi_{m'}^{l'}\rangle$ (taking into account only angular part)

$$\langle\Psi_m^l|r_{12}^{-1}|\Psi_{m'}^{l'}\rangle=(-1)^{m-m'}\sum_\mu(-1)^\mu\overline{g_\mu^l(r_1,r_2,\theta_{12})}g_{\mu+m-m'}^{l'}(r_1,r_2,\theta_{12})$$
$$\times\sum_k\frac{r_<^k}{r_>^{k+1}}\sum_K\sum_{Q=\text{even}}i^{-K}\begin{bmatrix}k&k&K\\0&0&0\end{bmatrix}\sum_{\bar{L}}\int_{S^2}d\hat{x}\,C_Q^K(\hat{x})\mathscr{S}_{0Q}^{\bar{L}}(\hat{x};+)$$
$$\times\sum_L\begin{bmatrix}k&k&K\\m-m'&Q+m'-m&Q\end{bmatrix}\begin{bmatrix}l&k&L\\-m&m-m'&-m'\end{bmatrix}\begin{bmatrix}L&l'&\bar{L}\\-m'&m'&0\end{bmatrix}$$
$$\times\begin{bmatrix}l&k&L\\-\mu&Q+m'-m&Q+m'-m-\mu\end{bmatrix}\begin{bmatrix}L&l'&\bar{L}\\Q+m'-m-\mu&m-m'+\mu&Q\end{bmatrix}.\qquad(48)$$

It is evident, this way of calculation is more efficient in comparison with direct integration of $\iint_{S^2}d\hat{x}_1 d\hat{x}_2\,\overline{D_{m\mu}^l(\Omega)}\left(C^k(\hat{x}_1)\cdot C^k(\hat{x}_2)\right)D_{m'\mu'}^{l'}(\Omega)$, because otherwise one should change integrands, when mapping from $\hat{x}$ to Ω. Consequently, that would lead to complex manipulations of trigonometric equations, given in Eq. (6).

7 Summary

In present study, we produced a parametrization of standard Wigner D-function on $SU(2)$ by the coordinates $(\hat{x}_1,\hat{x}_2)$ of vector in the fixed and rotated coordinate systems. As a result, we found the set of spherical functions, conformed to $D(\Omega)$ in miscellaneous areas $L^2(\Omega)\subset S^2$. We showed that offered parametrization of $D(\Omega)$ provides an opportunity to reduce angular $2N$-integrals, which are of special interest in theoretical atomic spectroscopy, to a double one. Particularly, we demonstrated a new way of construction of irreducible tensor operator

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matrix element, which plays the role of a generalization of previously obtained special cases (see, for example, Eq. (45)). Another convenient usage of suggested RCGC technique, based on coordinate transformation, is applied to the calculation of matrix elements on the basis of functions, expressed in terms of standard $D(\Omega)$ functions (for two-electron case, see Sec. 6.2).

A Optimal values for Ψ

Here the solutions $\Omega = (\varphi + \pi/2, \theta, \Psi) \in \mathbb{R} \; \forall \hat{x}_i \in S^2$ of Eq. (6) will be studied in a more detail. Partial solutions of the systems (x_2, z_2) and (y_2, z_2) for θ, φ are

$$\theta_{\sigma_1\sigma_2} = \sigma_1 \arccos \frac{z_1 z_2 + \sigma_2 |y_1'| \sqrt{z_1^2 - z_2^2 + y_1'^2}}{z_1^2 + y_1'^2} + 2\pi n_1, \, n_1 \in \mathbb{Z}^+, \tag{49}$$

$$\varphi_{\sigma_3\sigma_4}^{(1)} = \sigma_3 \arccos \frac{x_1' y_2 + \sigma_4 |x_2| \sqrt{1 - x_1'^2 - z_2^2}}{1 - z_2^2} + 2\pi n_2, \, n_2 \in \mathbb{Z}^+, \tag{50}$$

$$\varphi_{\sigma_3\sigma_4}^{(2)} = \sigma_3 \arccos \frac{x_2 \sqrt{1 - x_1'^2 - z_2^2} + \sigma_4 |x_1' y_2|}{\text{sgn}(y_1')(1 - z_2^2)} + 2\pi n_2, \, n_2 \in \mathbb{Z}^+, \tag{51}$$

where $\sigma_i \in \{-1, +1\}$; $\text{sgn}(y_1')$ denotes the sign of y_1'. Let us mark the common values of $\varphi_{\sigma_3\sigma_4}^{(1)}$ and $\varphi_{\sigma_3\sigma_4}^{(2)}$ by $\varphi_{\sigma_3\sigma_4} = {}_{n_2}\mathbf{w}_{\sigma_3\sigma_4}(\hat{x}_1, \hat{x}_2; \Psi)$. Let us also denote

$$\sin^2 \frac{\theta_{\sigma_1\sigma_2}}{2} = \mathbf{x}_{\sigma_2}(\hat{x}_1, \hat{x}_2; \Psi) = \frac{z_1^2 - z_1 z_2 + y_1'^2 + \sigma_2 y_1' \sqrt{z_1^2 - z_2^2 + y_1'^2}}{2(z_1^2 + y_1'^2)}. \tag{52}$$

Obtained functions $\mathbf{x}$ and $\mathbf{w}$ are substituted in Eq. (2). The generalized spherical function D is rearranged to the following function

$$\left\{ {}_{n_2}Z_{qq'}^k(\hat{x}_1, \hat{x}_2; \Psi) \right\}_{\sigma_2\sigma_3\sigma_4} = a(k, q, q') e^{iq\left(\frac{\pi}{2} + {}_{n_2}\mathbf{w}_{\sigma_3\sigma_4}(\hat{x}_1, \hat{x}_2; \Psi)\right) + iq'\Psi} \sum_p b_p(k, q, q')$$

$$\times \mathbf{x}_{\sigma_2}^{p - \frac{q-q'}{2}}(\hat{x}_1, \hat{x}_2; \Psi)(1 - \mathbf{x}_{\sigma_2}(\hat{x}_1, \hat{x}_2; \Psi))^{-p+k+\frac{q-q'}{2}}. \tag{53}$$

In order to look for optimal Ψ values, we carry out variational procedure for the gauge Ψ, applying it for all possible distributions of $\sigma_2, \sigma_3, \sigma_4$, i.e., $(\delta/\delta\Psi) {}_{n_2}Z_{qq'}^k = 0$. This implies

$$i {}_{n_2}Z_{qq'}^k \left(q' + q \frac{\delta {}_{n_2}\mathbf{w}_{\sigma_3\sigma_4}}{\delta\Psi} \right) + a e^{iq\left(\frac{\pi}{2} + {}_{n_2}\mathbf{w}_{\sigma_3\sigma_4}\right) + iq'\Psi} \sum_p b_p \frac{\delta \mathbf{x}_{\sigma_2}}{\delta\Psi}$$

$$\times \mathbf{x}_{\sigma_2}^{p - \frac{q-q'}{2} - 1}(1 - \mathbf{x}_{\sigma_2})^{-p+k+\frac{q-q'}{2}-1} \left(p - \frac{q-q'}{2} - k\mathbf{x}_{\sigma_2} \right) = 0. \tag{54}$$

Applying obvious fact, that $A = B = 0$ if $A, B \in \mathbb{R}$ in $A + iB = 0$, we finally gain

$$\begin{cases} \frac{\delta \mathbf{x}_{\sigma_2}}{\delta\Psi} = 0, \\ \mathbf{x}_{\sigma_2} = \eta, \, \eta \in \{0, 1, \frac{q'-q}{2k}\}, \\ q' + q \frac{\delta {}_{n_2}\mathbf{w}_{\sigma_3\sigma_4}}{\delta\Psi} = 0, q \neq 0. \end{cases} \tag{55}$$

It follows from equation $\mathbf{x}_{\sigma_2} = \eta$, that $y_1' \in \mathbb{C}$. Thus, Ψ does not belong to $\mathbb{R}$. Equation $\frac{\delta \mathbf{x}_{\sigma_2}}{\delta\Psi} = 0$ is rewritten in the form

$$\frac{\delta \mathbf{x}_{\sigma_2}}{\delta\Psi} = \frac{\delta \mathbf{x}_{\sigma_2}}{\delta y_1'} \frac{\delta y_1'}{\delta\Psi} = \frac{\delta \mathbf{x}_{\sigma_2}}{\delta y_1'} x_1' = 0. \tag{56}$$

The solutions of $\frac{\delta \mathbf{x}_+}{\delta y_1'} = 0$ for y_1' do not belong to $\mathbb{R}$. Thus, equation $x_1' = 0$ has to be solved. The latter is equivalent to Eq. (9). Finally, when studying the third equation in Eq. (55), we would get some individual values of Ψ, which depend on q, q' (for $q = 0$, present equation vanishes). Thus, the set of solutions would be the subset of solutions given by the first equation, independent of q, q'.

B The alternative expressions of spherical functions

In accordance with Eqs. (3)-(4), the product of coefficients a and b_p can be rewritten as follows

$$a\left(k,q,q'\right)b_p\left(k,q,q'\right) = \mathrm{i}^{q'-q}(-1)^p \left[\frac{(k+q)!\,(k-q)!}{(k+q')!\,(k-q')!}\right]^{\frac{1}{2}} \binom{k-q'}{p}\binom{k+q'}{p+q'-q}, \tag{57}$$

where the last two quantities on the right hand side of Eq. (57) denote binomial coefficients. Further, let us mark the term

$$A_{qq'}^k(\gamma) = a\left(k,q,q'\right)\left\{\cos\left[\tfrac{1}{2}\left(\theta_1 - \gamma\theta_2\right)\right]\right\}^{2k} \sum_p b_p\left(k,q,q'\right)\left\{\tan\left[\tfrac{1}{2}\left(\theta_1 - \gamma\theta_2\right)\right]\right\}^{2p+q'-q}. \tag{58}$$

According to Eq. (57), $A_{qq'}^k(\gamma)$ may be revised by

$$A_{qq'}^k(\gamma) = \mathrm{i}^{q'-q}\left[\frac{(k+q)!\,(k-q)!}{(k+q')!\,(k-q')!}\right]^{\frac{1}{2}} \sum_p (-1)^p \binom{k-q'}{p}\binom{k+q'}{p+q'-q} \frac{z^{p+\frac{q'-q}{2}}}{(1+z)^k}, \tag{59}$$

where $z = \tan^2\left[\tfrac{1}{2}\left(\theta_1 - \gamma\theta_2\right)\right]$. Performing the summation over p, we obtain

$$\sum_p (-1)^p \binom{k-q'}{p}\binom{k+q'}{p+q'-q} \frac{z^{p+\frac{q'-q}{2}}}{(1+z)^k}$$

$$= (-1)^{q-q'} \binom{k-q'}{q-q'} z^{\frac{q-q'}{2}} (1+z)^{1+k}\, {}_2F_1\left(k+1+q, k+1-q'; 1+q-q'; -z\right) \quad (q \geq q') \tag{60a}$$

$$= \binom{k+q'}{q'-q} z^{\frac{q'-q}{2}} (1+z)^{1+k}\, {}_2F_1\left(k+1+q', k+1-q; 1+q'-q; -z\right) \quad (q' \geq q). \tag{60b}$$

Thus if: (a) $A_{qq'}^{>k} = A_{qq'}^k$, for $q \geq q'$; (b) $A_{qq'}^{<k} = A_{qq'}^k$, for $q' \geq q$, then

$$A_{qq'}^{>k}(\gamma) = \frac{\mathrm{i}^{q-q'}}{(q-q')!}\left[\frac{(k+q)!\,(k-q')!}{(k+q')!\,(k-q)!}\right]^{\frac{1}{2}} \left\{\tan\left[\tfrac{1}{2}\left(\theta_1 - \gamma\theta_2\right)\right]\right\}^{q-q'} \left\{\cos\left[\tfrac{1}{2}\left(\theta_1 - \gamma\theta_2\right)\right]\right\}^{-2-2k}$$

$$\times {}_2F_1\left(k+1+q, k+1-q'; 1+q-q'; -\tan^2\left[\tfrac{1}{2}\left(\theta_1 - \gamma\theta_2\right)\right]\right), \tag{61}$$

$$A_{qq'}^{<k}(\gamma) = A_{q'q}^{>k}(\gamma). \tag{62}$$

Substituting A in Eq. (15) we gather

$$\left(n, n'; \alpha, \beta, \gamma, \delta | \hat{x}_1, \hat{x}_2\right)_{qq'}^k = \begin{cases} \left(n, n'; \alpha, \beta, \gamma, \delta | \hat{x}_1, \hat{x}_2\right)_{qq'}^{>k}, & q \geq q', \\ \left(n, n'; \alpha, \beta, \gamma, \delta | \hat{x}_1, \hat{x}_2\right)_{qq'}^{<k}, & q \leq q', \end{cases} \tag{63}$$

$$\left(n, n'; \alpha, \beta, \gamma, \delta | \hat{x}_1, \hat{x}_2\right)_{qq'}^{>k} = \mathrm{i}^{\alpha q + \delta q'}(-1)^{2\left(nk+n'q'\right)}\beta^{q'-q}\mathrm{e}^{\mathrm{i}\left(q\varphi_2 - q'\varphi_1\right)} A_{qq'}^{>k}(\gamma), \tag{64}$$

$$\left(n, n'; \alpha, \beta, \gamma, \delta | \hat{x}_1, \hat{x}_2\right)_{qq'}^{<k} = \mathrm{i}^{(\alpha-\delta)\left(q-q'\right)}\mathrm{e}^{\mathrm{i}\left(\varphi_1 + \varphi_2\right)\left(q-q'\right)} \left(n, n'; \alpha, \beta, \gamma, \delta | \hat{x}_1, \hat{x}_2\right)_{q'q}^{>k}. \tag{65}$$

C Reduced matrix element on the basis of spherical harmonics

Here a proof of Eq. (45), exploiting RCGC technique, will be offered. The matrix element of $T_q^k(\hat{x})$ on the basis of arbitrary functions $\psi_m^{l\dagger}(\hat{x})$ and $\psi_{\bar{m}}^{\bar{l}}(\hat{x})$ is written by

$$\langle lm|T_q^k|\bar{l}\bar{m}\rangle = [l\|T^k\|\bar{l}] \begin{bmatrix} \bar{l} & k & l \\ \bar{m} & q & m \end{bmatrix} = \int_{S^2} \mathrm{d}\hat{x}\, \psi_m^{l\dagger}(\hat{x}) T_q^k(\hat{x}) \psi_{\bar{m}}^{\bar{l}}(\hat{x}). \tag{66}$$

Direct adaptation of Eq. (24) points to

$$\langle lm|T_q^k|\bar{l}\bar{m}\rangle = \int_{S^2} \mathrm{d}\hat{x} \sum_{m'q'\bar{m}'} \psi_{m'}^{l\dagger}(\hat{x}') T_{q'}^k(\hat{x}') \psi_{\bar{m}'}^{\bar{l}}(\hat{x}') \overline{\eta_{mm'}^l(\hat{x}',\hat{x})} \eta_{qq'}^k(\hat{x}',\hat{x}) \eta_{\bar{m}\bar{m}'}^{\bar{l}}(\hat{x}',\hat{x}). \tag{67}$$

Transformed functions ψ and operator T depend on fixed coordinates $\hat{x}'$. Consequently, they can be located in front of the integral. Recalling, that $\overline{\eta_{mm'}^l} = (-1)^{m-m'}\eta_{-m-m'}^l$, and exploiting reduction rules for the Kronecker products $l \times k \to \bar{L}$, $\bar{L} \times \bar{l} \to L$ (see Eq. (26)), we attain $\eta_{MM'}^L(\hat{x}',\hat{x})$. The integral of present spherical function is defined in Eq. (29), and in this case equals to $\mathscr{S}_{0M'}^L(\hat{x}';+)$ (see Eq. (39)), since $L \in \mathbb{Z}^+$. Thus

$$\langle lm|T_q^k|\bar{l}\bar{m}\rangle = \sum_{m'q'\bar{m}'} (-1)^{m-m'} \psi_{m'}^{l\dagger}(\hat{x}') T_{q'}^k(\hat{x}') \mathscr{S}_{0M'}^L(\hat{x}';+) \psi_{\bar{m}'}^{\bar{l}}(\hat{x}')$$

$$\times \begin{bmatrix} l & k & \bar{L} \\ -m & q & -\bar{m} \end{bmatrix} \begin{bmatrix} l & k & \bar{L} \\ -m' & q' & \bar{M}' \end{bmatrix} \begin{bmatrix} \bar{L} & \bar{l} & L \\ -\bar{m} & \bar{m} & 0 \end{bmatrix} \begin{bmatrix} \bar{L} & \bar{l} & L \\ \bar{M}' & \bar{m}' & M' \end{bmatrix}. \tag{68}$$

The matrix element does not depend on $\hat{x}'$, thus one can choose any value. We select the most simple case $\hat{x}' = \hat{0} \equiv (0,0)$. The application of orthogonality condition for Clebsh-Gordan coefficients, combining Eqs. (66), (68), leads to equalities $\bar{L} = \bar{l}$, $L = 0$; thus $\mathscr{S}_{00}^0(\hat{0};+) = 4\pi$ and

$$[l\|T^k\|\bar{l}] = \frac{4\pi}{2l+1} \sum_{m'q'\bar{m}'} \psi_{m'}^{l\dagger}(\hat{0}) T_{q'}^k(\hat{0}) \psi_{\bar{m}'}^{\bar{l}}(\hat{0}) \begin{bmatrix} \bar{l} & k & l \\ \bar{m}' & q' & m' \end{bmatrix}. \tag{69}$$

It is noticeable, obtained expression, by applying technique of coordinate transformations, coincides with Eq. (41) in [8], if reducing given Kronecker products $l \times k \to L'$, $L' \times \bar{l} \to L''$. This would signify $L' = \bar{l}$ and $L'' = 0$. At this step we turn to special case of eigenfunctions $\psi_m^l(\hat{x}) = Y_m^l(\hat{x})$, what implies equality $Y_m^l(\hat{0}) = \delta_{m0}\mathrm{i}^l\sqrt{(2l+1)/4\pi}$. Hence Eq. (69) becomes equal to expression, presented in Eq. (45). One should be also reminded, that in general, in Eq. (69) the arguments $\hat{0}$ can be replaced by any values $\hat{x}$.

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